

=> FILE REG

FILE 'REGISTRY' ENTERED AT 14:59:12 ON 14 AUG 2003  
USE IS ~~SUBJECT~~ TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2003 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file  
provided by InfoChem.

STRUCTURE FILE UPDATES: 13 AUG 2003 HIGHEST RN 566135-25-9  
DICTIONARY FILE UPDATES: 13 AUG 2003 HIGHEST RN 566135-25-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP  
PROPERTIES for more information. See STNote 27, Searching Properties  
in the CAS Registry File, for complete details:  
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> FILE HCAPLU

FILE 'HCAPLUS' ENTERED AT 14:59:16 ON 14 AUG 2003  
USE IS ~~SUBJECT~~ TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is  
held by the publishers listed in the PUBLISHER (PB) field (available  
for records published or updated in Chemical Abstracts after December  
26, 1996), unless otherwise indicated in the original publications.  
The CA Lexicon is the copyrighted intellectual property of the  
the American Chemical Society and is provided to assist you in searching  
databases on STN. Any dissemination, distribution, copying, or storing  
of this information, without the prior written consent of CAS, is  
strictly prohibited.

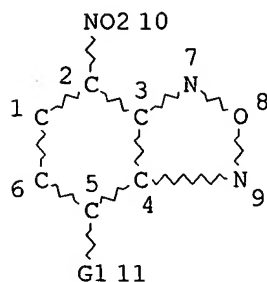
FILE COVERS 1907 - 14 Aug 2003 VOL 139 ISS 7  
FILE LAST UPDATED: 13 Aug 2003 (20030813/ED)

This file contains CAS Registry Numbers for easy and accurate  
substance identification.

=> D QUE

L25

STR



*1688 structures from query*

VAR G1=O/S/N  
 NODE ATTRIBUTES:  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE

L27 1688 SEA FILE=REGISTRY SSS FUL L25  
 L28 1108 SEA FILE=HCAPLUS ABB=ON L27  
 L32 9 SEA FILE=HCAPLUS ABB=ON L28 AND (SILK OR WOOL OR FUR OR HAIR  
 OR KERAT?)

=> D L32 ALL 1-9 HITSTR

*9 CA references with ability*

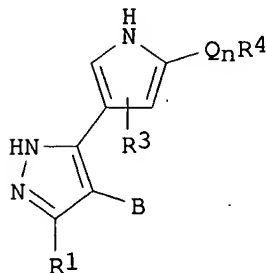
L32 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2003 ACS on STN  
 AN 2003:117818 HCAPLUS  
 DN 138:153530  
 TI Preparation of pyrazolylpyrrolicarboxamides as protein kinase inhibitors  
 IN Tang, Qing; Maltais, Francois; Janetka, James Walter; Hale, Michael Robin  
 PA Vertex Pharmaceuticals Incorporated, USA  
 SO PCT Int. Appl., 66 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 IC ICM C07D401-04  
 ICS C07D405-14; C07D401-14; C07D403-14; C07D413-14; A61K031-4155;  
 A61K031-4439; A61P035-00; A61P029-00  
 CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 1

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003011854	A1	20030213	WO 2002-US24723	20020802
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,				

CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,  
PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,  
NE, SN, TD, TG

US 2003139452 A1 20030724 US 2002-212292 20020802  
PRAI US 2001-309886P P 20010803  
OS MARPAT 138:153530  
GI



- AB Title compds. [I; B = substituted aryl, heteroaryl, heterocyclyl; Q = (substituted) alkylidene; n = 0, 1; R1 = H, F, R, N(R7)2, OR7, NR7COR7, NR7SO2R7, etc.; R3 = H, R, OH, OR, N(R7)2, F, cyano; R4 = (CH2)yR6, N(R5)2, etc.; R = (substituted) aliph., aryl, heteroaryl, heterocyclyl; R5 = R, (CH2)yR6, R7, CON(R7)2, SO2R7, etc.; y = 0-6; R6 = H, R, (CH2)yR, OH, OR, CO2R, N(R7)2, etc.; R7 = H, (substituted) aliph.; N(R7)2 = 5-8 membered heterocyclyl, heteroaryl], were prepd. Thus, Ac-hydroxyproline-OH was stirred with HOBT and EDCI in DMF; 4-[4-(4-aminomethyl-3-chlorophenyl)-1H-pyrazol-3-yl]-1H-pyrrole-2-carboxylic acid [1-(3-chloro-4-fluorophenyl)-2-hydroxyethyl]amide (prepn. given) and triethylamine were added followed by stirring for 2 h to give 4-[4-[4-[(1-acetyl-4-hydroxypyrrolidine-2-carbonyl)amino]methyl]-3-chlorophenyl]-1H-pyrazol-3-yl]-1H-pyrrole-2-carboxylic acid [1-(3-chloro-4-fluorophenyl)-2-hydroxyethyl]amide. The latter inhibited ERK2 with  $K_i < 1 \mu\text{M}$ . I are useful for treating disease states in mammals that are alleviated by a protein kinase inhibitor, particularly diseases such as cancer, inflammatory disorders, restenosis, and cardiovascular disease.
- ST pyrazolylpyrrolecarboxamide prepn protein kinase inhibitor; ERK2 AKT kinase inhibitor pyrazolylpyrrolecarboxamide prepn; cancer diabetes hepatomegaly cardiovascular disease treatment; alzheimers disease cystic fibrosis viral disease treatment pyrazolylpyrrolecarboxamide
- IT Lung, neoplasm  
(adenocarcinoma, treatment; prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)
- IT Platelet (blood)  
(aggregation, treatment; prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)
- IT Nervous system, disease  
(amyotrophic lateral sclerosis, treatment; prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)
- IT Antiarteriosclerotics  
(antiatherosclerotics; prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)

- IT Bladder, neoplasm  
(carcinoma, treatment; prepn. of pyrazolylpyrrolecaboxamides as protein kinase inhibitors)
- IT Nervous system, disease  
Nervous system, neoplasm  
(central, treatment; prepn. of pyrazolylpyrrolecaboxamides as protein kinase inhibitors)
- IT Uterus, neoplasm  
(cervix, treatment; prepn. of pyrazolylpyrrolecaboxamides as protein kinase inhibitors)
- IT Leukemia  
(chronic myelocytic, treatment; prepn. of pyrazolylpyrrolecaboxamides as protein kinase inhibitors)
- IT Intestine, neoplasm  
(colon, treatment; prepn. of pyrazolylpyrrolecaboxamides as protein kinase inhibitors)
- IT Intestine, neoplasm  
(colorectal, treatment; prepn. of pyrazolylpyrrolecaboxamides as protein kinase inhibitors)
- IT Artery, disease  
(coronary, restenosis, treatment; prepn. of pyrazolylpyrrolecaboxamides as protein kinase inhibitors)
- IT Urogenital tract  
(disease, cancer treatment; prepn. of pyrazolylpyrrolecaboxamides as protein kinase inhibitors)
- IT Immunity  
(disorder, treatment; prepn. of pyrazolylpyrrolecaboxamides as protein kinase inhibitors)
- IT Thyroid gland, neoplasm  
(follicular cell carcinoma, treatment; prepn. of pyrazolylpyrrolecaboxamides as protein kinase inhibitors)
- IT Neuroglia, neoplasm  
(glioblastoma, treatment; prepn. of pyrazolylpyrrolecaboxamides as protein kinase inhibitors)
- IT Leukemia  
(hairy-cell, treatment; prepn. of pyrazolylpyrrolecaboxamides as protein kinase inhibitors)
- IT Liver, disease  
(hepatomegaly, treatment; prepn. of pyrazolylpyrrolecaboxamides as protein kinase inhibitors)
- IT Heart, disease  
(hypertrophy, treatment; prepn. of pyrazolylpyrrolecaboxamides as protein kinase inhibitors)
- IT Heart, disease  
(infarction, treatment; prepn. of pyrazolylpyrrolecaboxamides as protein kinase inhibitors)
- IT Brain, disease  
(ischemia, treatment; prepn. of pyrazolylpyrrolecaboxamides as protein kinase inhibitors)
- IT Skin, neoplasm  
(keratoacanthoma, treatment; prepn. of pyrazolylpyrrolecaboxamides as protein kinase inhibitors)
- IT Lung, neoplasm  
(large-cell carcinoma, treatment; prepn. of pyrazolylpyrrolecaboxamides as protein kinase inhibitors)
- IT Hematopoietic precursor cell  
(myeloid, cancer treatment; prepn. of pyrazolylpyrrolecaboxamides as protein kinase inhibitors)

IT Nerve, neoplasm  
(neuroblastoma, treatment; prepn. of pyrazolylpyrrolicarboxamides as protein kinase inhibitors)

IT Thyroid gland, neoplasm  
(papillary carcinoma, treatment; prepn. of pyrazolylpyrrolicarboxamides as protein kinase inhibitors)

IT Allergy inhibitors  
Anti-Alzheimer's agents  
Anti-infective agents  
Anti-inflammatory agents  
Antitumor agents  
Human  
Platelet aggregation inhibitors  
(prepn. of pyrazolylpyrrolicarboxamides as protein kinase inhibitors)

IT Kidney, neoplasm  
(renal cell carcinoma, treatment; prepn. of pyrazolylpyrrolicarboxamides as protein kinase inhibitors)

IT Testis, neoplasm  
(seminoma, treatment; prepn. of pyrazolylpyrrolicarboxamides as protein kinase inhibitors)

IT Lung, neoplasm  
(small-cell carcinoma, treatment; prepn. of pyrazolylpyrrolicarboxamides as protein kinase inhibitors)

IT Carcinoma  
(squamous cell, treatment; prepn. of pyrazolylpyrrolicarboxamides as protein kinase inhibitors)

IT Brain, disease  
(stroke, treatment; prepn. of pyrazolylpyrrolicarboxamides as protein kinase inhibitors)

IT Adenoma  
Allergy  
Alzheimer's disease  
Antiviral agents  
Atherosclerosis  
Autoimmune disease  
Biliary tract, neoplasm  
Bone, disease  
Bone, neoplasm  
Brain, neoplasm  
Cardiovascular system, disease  
Cell death  
Cystic fibrosis  
Diabetes mellitus  
Endocrine system, disease  
Esophagus, neoplasm  
Hodgkin's disease  
Immunodeficiency  
Infection  
Inflammation  
Intestine, neoplasm  
Larynx, neoplasm  
Leukemia  
Liver, disease  
Liver, neoplasm  
Lung, neoplasm  
Lymphoma  
Mammary gland, neoplasm  
Melanoma

Mouth, neoplasm  
Neoplasm  
Nervous system, disease  
Ovary, neoplasm  
Pancreas, neoplasm  
Pharynx, neoplasm  
Prostate gland, neoplasm  
Psoriasis  
Sarcoma  
Skin, neoplasm  
Stomach, neoplasm  
Testis, neoplasm  
Thyroid gland, neoplasm  
Transplant and Transplantation

(treatment; prepn. of pyrazolylpyrrolicarboxamides as protein kinase inhibitors)

IT Carcinoma

(undifferentiated, treatment; prepn. of pyrazolylpyrrolicarboxamides as protein kinase inhibitors)

IT 137632-08-7, Erk2 kinase 148640-14-6

RL: BSU (Biological study, unclassified); BIOL (Biological study)

(inhibitors; prepn. of pyrazolylpyrrolicarboxamides as protein kinase inhibitors)

IT 496856-34-9P 496856-35-0P 496856-36-1P 496856-37-2P 496856-38-3P  
496856-39-4P 496856-40-7P **496856-41-8P** 496856-42-9P  
496856-43-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of pyrazolylpyrrolicarboxamides as protein kinase inhibitors)

IT 5414-19-7, 2-Bromoethyl ether 7216-42-4, 4-Pyridinecarboxaldehyde  
N-oxide 33697-81-3, 3-Chloro-4-hydroxyphenylacetic acid 33996-33-7,  
N-Acetylhydroxyproline 35302-72-8, 2-(Trichloroacetyl)pyrrole  
496856-51-0 496856-52-1

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of pyrazolylpyrrolicarboxamides as protein kinase inhibitors)

IT 57017-95-5P, Methyl 3-chloro-4-hydroxyphenylacetate 496856-44-1P  
496856-45-2P 496856-46-3P 496856-47-4P 496856-48-5P 496856-49-6P  
496856-50-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of pyrazolylpyrrolicarboxamides as protein kinase inhibitors)

RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

- (1) Ambiter; Screening Collection (Catalog) 1999
- (2) Anantanarayan; US 5932576 A 1999 HCAPLUS
- (3) Davis; US 5922741 A 1999 HCAPLUS
- (4) G D Searle & Co; WO 9852941 A 1998 HCAPLUS
- (5) Vertex Pharmaceuticals; WO 0156993 A 2001 HCAPLUS
- (6) Vertex Pharmaceuticals; WO 0157022 A 2001 HCAPLUS
- (7) Vertex Pharmaceuticals; WO 0222610 A 2002 HCAPLUS

IT **496856-41-8P**

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of pyrazolylpyrrolicarboxamides as protein kinase inhibitors)

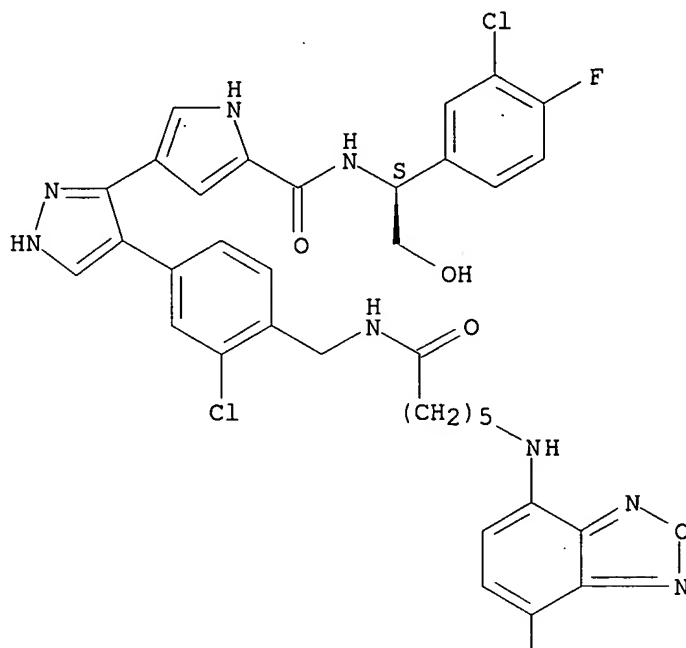
RN 496856-41-8 HCAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-1-(3-chloro-4-fluorophenyl)-2-

hydroxyethyl]-4-[4-[3-chloro-4-[[6-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]-1-oxohexyl]amino]methyl]phenyl]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A

 $\text{NO}_2$ 

L32 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2003 ACS on STN

AN 2002:733871 HCAPLUS

DN 137:252675

TI Two-component direct **hair** dyes

IN Umbricht, Gisela; Braun, Hans-Juergen; Oberson, Sylviane; Mueller, Catherine

PA Wella AG, Germany

SO Ger. Offen., 12 pp.

CODEN: GWXXBX

DT Patent

LA German

IC ICM A61K007-13

CC 62-3 (Essential Oils and Cosmetics)

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 10114426	A1	20020926	DE 2001-10114426	20010324

PRAI DE 2001-10114426 20010324

OS MARPAT 137:252675

AB The invention concerns direct **hair** dyes that are composed of two dyes; component A1 contains benzodiazole, benzothiazole, benzoselenadiazole derivs.; component A2 is selected from the group of aliph. esters, indolium, quinolinium, pyrazole, pyrazolinone, furan, etc. derivs. Thus component A1 contained (g): 7-chloro-4-nitro-2,1,3-benzoxadiazole 0.25; ethanol 5.00; Plantaren 2000 4.00; EDTA disodium hydrate 0.20; water to 100. Component A2 was 0.22 g 1-phenyl-3-methyl-5-pyrazolone. The components were mixed and sodium carbonate was added; the pH was set to desired value with sodium hydroxide and the mixt. was applied to **hair**.

ST direct **hair** dye two component sodium carbonate

IT pH

(two-component direct **hair** dyes)

IT 59-48-3, Oxindole 67-52-7, Barbituric acid 89-25-8,  
1-Phenyl-3-methyl-5-pyrazolone 105-34-0, Acetic acid, cyano-, methyl  
ester 105-53-3, Malonic acid diethyl ester 105-56-6, Acetic acid,  
cyano-, ethyl ester 107-91-5, 2-Cyanoacetamide 108-26-9 108-59-8,  
Malonic acid dimethyl ester 109-77-3, Malonic acid dinitrile 118-12-7,  
1,3,3-Trimethyl-2-methyleneindoline 141-84-4, Rhodanine 372-09-8  
497-19-8, Sodium carbonate, biological studies 504-02-9,  
Cyclohexane-1,3-dione 504-17-6, Thiobarbituric acid 541-50-4D,  
Acetoacetic acid, esters 553-86-6, Cumaranone 606-23-5, 1,3-Indandione  
606-55-3 608-08-2, 3-Indoxylacetate 876-87-9 939-83-3 1753-20-4  
2160-10-3 2207-29-6 2274-63-7 2274-89-7 2654-52-6 2749-59-9  
2785-06-0 3158-63-2, 1,3-Dimethylthiobarbituric acid 3524-07-0  
5418-63-3, 1,2,3,3-Tetramethyl-3H-indoliumiodide 5714-17-0 5718-83-2,  
Rhodanine-3-acetic acid 6583-06-8 10199-89-0, 7-Chloro-4-nitro-2,1,3-  
benzoxadiazole 15639-38-0 15639-43-7 15944-78-2 16322-19-3,  
4-Nitro-2,1,3-benzoxadiazole 16859-86-2, 1,4-Dimethylquinoliniumiodide  
18333-71-6 **18333-73-8**, 2,1,3-Benzoxadiazole, 4-methoxy-7-nitro-  
18378-23-9 18392-74-0 18392-77-3 18453-42-4 19951-28-1  
19951-33-8 19951-34-9 20718-28-9 20718-41-6 20718-46-1  
20718-47-2 20718-48-3 26460-78-6 26738-24-9 29270-56-2,  
2,1,3-Benzoxadiazole, 4-fluoro-7-nitro- 30536-22-2 32051-92-6  
35128-56-4, 2,1,3-Benzoxadiazole, 4-bromo-7-nitro- 41927-50-8  
52120-98-6 59997-51-2, Pivaloylacetonitrile 61224-35-9,  
1,2,3,3-Tetramethyl-3H-indolium-p-toluene sulfonate 68579-76-0  
70264-71-0 72023-79-1 **81432-10-2**, 2,1,3-Benzoxadiazole,  
4-ethoxy-7-nitro- 89365-28-6 89365-31-1 89365-32-2 89793-80-6  
89793-88-4 90841-38-6 91267-92-4 91330-69-7 91760-88-2  
100181-80-4 125292-42-4 131202-67-0 131202-71-6 227199-11-3  
257932-06-2 257932-07-3 404839-62-9 404839-63-0 404839-64-1  
413612-09-6 460987-45-5 460987-46-6 460987-47-7 460987-48-8  
460987-49-9 460987-50-2 460987-52-4

RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)

(two-component direct **hair** dyes)IT **18333-73-8**, 2,1,3-Benzoxadiazole, 4-methoxy-7-nitro-**81432-10-2**, 2,1,3-Benzoxadiazole, 4-ethoxy-7-nitro-

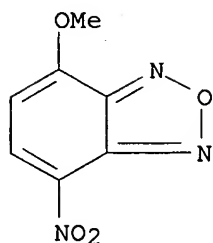
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)

(two-component direct **hair** dyes)

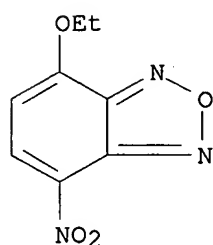
RN 18333-73-8 HCAPLUS

CN 2,1,3-Benzoxadiazole, 4-methoxy-7-nitro- (9CI) (CA INDEX NAME)





RN 81432-10-2 HCAPLUS  
 CN 2,1,3-Benzoxadiazole, 4-ethoxy-7-nitro- (9CI) (CA INDEX NAME)



L32 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2003 ACS on STN  
 AN 2002:220344 HCAPLUS  
 DN 136:267892  
 TI Use of 4-nitro-2,1,3-benzoxadiazole derivatives as **hair** dyes  
 IN Pasquier, Cecile; Charriere, Veronique; Braun, Hans-Juergen  
 PA Wella Aktiengesellschaft, Germany  
 SO PCT Int. Appl., 35 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA German  
 IC ICM A61K007-13  
 CC 62-3 (Essential Oils and Cosmetics)  
 Section cross-reference(s): 27, 41  
 FAN.CNT 1

*applicant*

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002022094	A1	20020321	WO 2001-EP7497	20010629
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
DE 10045599	A1	20020404	DE 2000-10045599	20000915
AU 2001069112	A5	20020326	AU 2001-69112	20010629
BR 2001007208	A	20020709	BR 2001-7208	20010629
EP 1317242	A1	20030611	EP 2001-947431	20010629

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

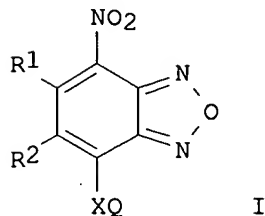
US 2002189032 A1 20021219 US 2002-89207 20020326

PRAI DE 2000-10045599 A 20000915

WO 2001-EP7497 W 20010629

OS MARPAT 136:267892

GI



AB The invention relates to the use of 4-nitro-benzo-2,1,3-oxadiazol derivs. of general formula (I) as dyes in coloring agents for **keratin** fibers, for example, **wool, silk, fur** or **hair** and particularly human **hair**. In formula I X represents oxygen, sulfur or NRa, Ra represents hydrogen, an (C1-C4) alkyl group, a monohydroxy (C1-C4) alkyl group, a polyhydroxy (C2-C4) alkyl group, a mono (C1-C4) alkoxy (C1-C4) alkyl group; R1 and R2 can be identical or different and represent independently from each other hydrogen, a halogen atom, an (C1-C4) alkyl group, an (C1-C4) alkyl group substituted by a halogen atom, an (C1-C4) alkoxy group, a nitro group or a NRbRc group, wherein the radicals Rb and Rc can be identical or different and represent independently from each other hydrogen, a (C1-C4) alkyl group, an optionally substituted arom. carbocycle or an (C1-C4) alkane carbonyl group, or Rb and Rc together with the nitrogen atom form a heterocyclic (C3-C6) group; Q represents hydrogen, an aliph. group, an arom. isocyclic group or an arom. heterocyclic group. Thus 7-nitro-4-(N-phenyl-amino)-2,1,3-benzodioxazole was synthesized and 2.5 mmol were used in a **hair** dye that further contained (g): ethanol 5; Plantaren 2000 4.0; EDTA sodium salt hydrate 0.2; water to 100.

ST nitro benzoxadiazole deriv **hair** dye

IT **Hair** preparations

(dyes; use of 4-nitro-2,1,3-benzoxadiazole derivs. as **hair** dyes)

IT **Fur**

**Silk**

**Wool**

(use of 4-nitro-2,1,3-benzoxadiazole derivs. as **hair** dyes)

IT **Keratins**

RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)

(use of 4-nitro-2,1,3-benzoxadiazole derivs. as **hair** dyes)

IT 1455-87-4 7722-84-1, Hydrogen peroxide, biological studies

10199-91-4, 4-Amino-7-nitro-2, 1,3-benzoxadiazole

16322-23-9 18378-17-1 18378-18-2

19155-64-7 53619-61-7 53619-62-8

53619-63-9 53619-64-0 73853-83-5

73853-84-6 81432-10-2 90786-92-8

90786-95-1 97346-17-3 101237-21-2  
101237-22-3 101237-23-4 101237-24-5  
101237-27-8 102565-92-4 118025-13-1  
121782-85-2 121782-87-4 121782-88-5  
121782-92-1 121782-93-2 126865-59-6  
126865-60-9 126865-61-0 126865-63-2  
155866-58-3 199727-69-0 199727-70-3  
199727-71-4 324525-87-3 404823-74-1  
404823-79-6 404823-80-9 404823-81-0  
404823-86-5 404823-87-6 404823-88-7  
404823-89-8

RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)  
(use of 4-nitro-2,1,3-benzoxadiazole derivs. as **hair** dyes)

IT 16597-10-7P 18333-73-8P 18378-15-9P

101237-25-6P 101237-26-7P 404823-73-0P

RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(use of 4-nitro-2,1,3-benzoxadiazole derivs. as **hair** dyes)

IT 62-53-3, Aniline, reactions 106-50-3, 1,4-Diaminobenzene, reactions  
108-95-2, Phenol, reactions 123-30-8, 4-Aminophenol 10199-89-0,  
4-Chloro-7-nitro-2,1,3-benzoxadiazole 93841-25-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(use of 4-nitro-2,1,3-benzoxadiazole derivs. as **hair** dyes)

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

- (1) Akademie der Wissenschaften der Ddr; DE 277678 C
- (2) Bachmann, H; US 4620850 A 1986 HCAPLUS
- (3) Henkel; WO 0147485 A 2001
- (4) Lim, M; US 5055110 A 1991 HCAPLUS
- (5) M Luther Universitat; DD 228900 A 1985 HCAPLUS

IT 1455-87-4 10199-91-4, 4-Amino-7-nitro-2,  
1,3-benzoxadiazole 16322-23-9 18378-17-1

18378-18-2 19155-64-7 53619-61-7

53619-62-8 53619-63-9 53619-64-0

73853-83-5 73853-84-6 81432-10-2

90786-92-8 90786-95-1 97346-17-3

101237-21-2 101237-22-3 101237-23-4

101237-24-5 101237-27-8 102565-92-4

118025-13-1 121782-85-2 121782-87-4

121782-88-5 121782-92-1 121782-93-2

126865-59-6 126865-60-9 126865-61-0

126865-63-2 155866-58-3 199727-69-0

199727-70-3 199727-71-4 324525-87-3

404823-74-1 404823-79-6 404823-80-9

404823-81-0 404823-86-5 404823-87-6

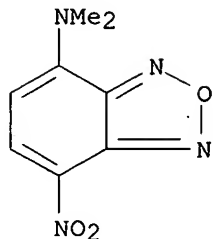
404823-88-7 404823-89-8

RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)

(use of 4-nitro-2,1,3-benzoxadiazole derivs. as **hair** dyes)

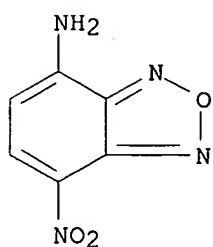
RN 1455-87-4 HCAPLUS

CN 2,1,3-Benzoxadiazol-4-amine, N,N-dimethyl-7-nitro- (9CI) (CA INDEX NAME)



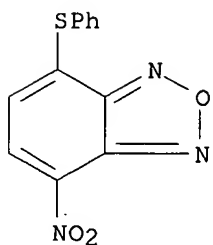
RN 10199-91-4 HCAPLUS

CN 2,1,3-Benzoxadiazol-4-amine, 7-nitro- (9CI) (CA INDEX NAME)



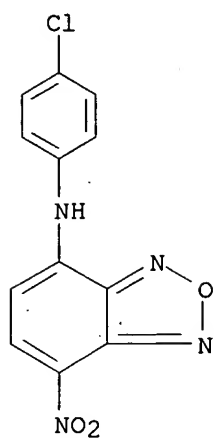
RN 16322-23-9 HCAPLUS

CN 2,1,3-Benzoxadiazole, 4-nitro-7-(phenylthio)- (9CI) (CA INDEX NAME)



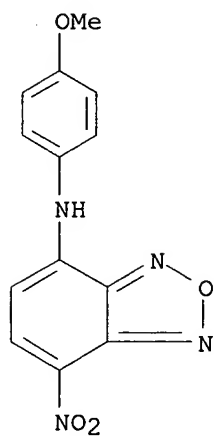
RN 18378-17-1 HCAPLUS

CN 2,1,3-Benzoxadiazol-4-amine, N-(4-chlorophenyl)-7-nitro- (9CI) (CA INDEX NAME)



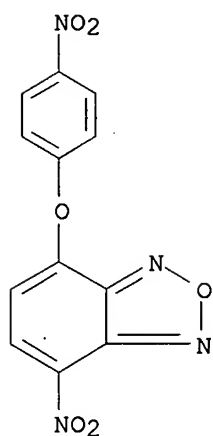
RN 18378-18-2 HCAPLUS

CN 2,1,3-Benzoxadiazol-4-amine, N-(4-methoxyphenyl)-7-nitro- (9CI) (CA INDEX NAME)



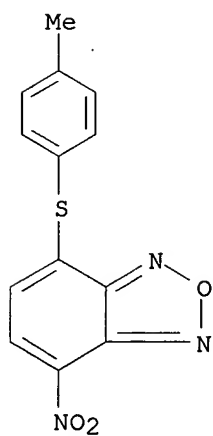
RN 19155-64-7 HCAPLUS

CN 2,1,3-Benzoxadiazole, 4-nitro-7-(4-nitrophenoxy)- (9CI) (CA INDEX NAME)



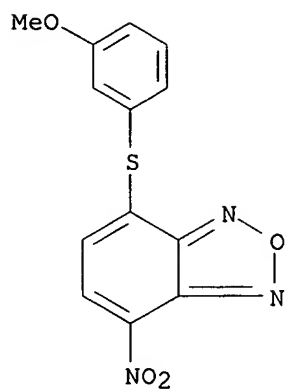
RN 53619-61-7 HCAPLUS

CN 2,1,3-Benzoxadiazole, 4-[(4-methylphenyl)thio]-7-nitro- (9CI) (CA INDEX NAME)



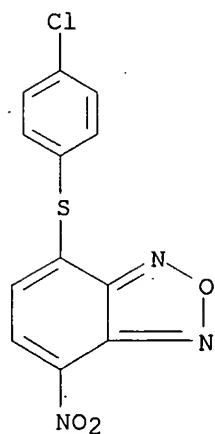
RN 53619-62-8 HCAPLUS

CN 2,1,3-Benzoxadiazole, 4-[(3-methoxyphenyl)thio]-7-nitro- (9CI) (CA INDEX NAME)



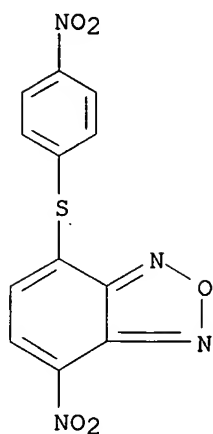
RN 53619-63-9 HCAPLUS

CN 2,1,3-Benzoxadiazole, 4-[(4-chlorophenyl)thio]-7-nitro- (9CI) (CA INDEX NAME)



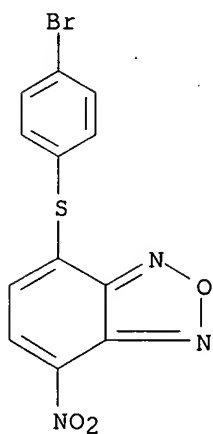
RN 53619-64-0 HCAPLUS

CN 2,1,3-Benzoxadiazole, 4-nitro-7-[(4-nitrophenyl)thio]- (9CI) (CA INDEX NAME)



RN 73853-83-5 HCAPLUS

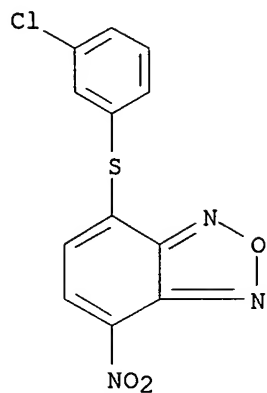
CN 2,1,3-Benzoxadiazole, 4-[(4-bromophenyl)thio]-7-nitro- (9CI) (CA INDEX NAME)



RN 73853-84-6 HCAPLUS

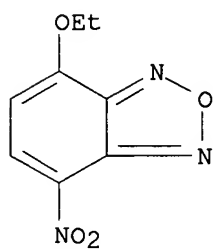
CN 2,1,3-Benzoxadiazole, 4-[(3-chlorophenyl)thio]-7-nitro- (9CI) (CA INDEX NAME)





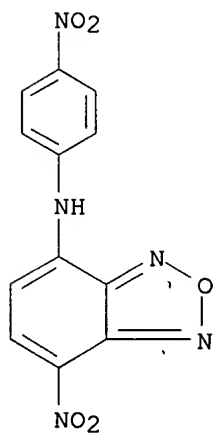
RN 81432-10-2 HCAPLUS

CN 2,1,3-Benzoxadiazole, 4-ethoxy-7-nitro- (9CI) (CA INDEX NAME)



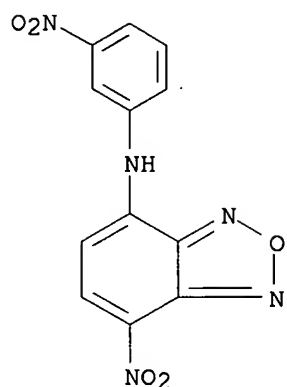
RN 90786-92-8 HCAPLUS

CN 2,1,3-Benzoxadiazol-4-amine, 7-nitro-N-(4-nitrophenyl)- (9CI) (CA INDEX NAME)



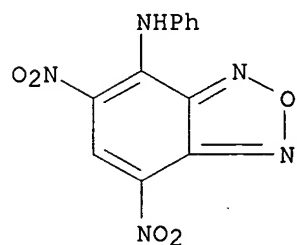
RN 90786-95-1 HCAPLUS

CN 2,1,3-Benzoxadiazol-4-amine, 7-nitro-N-(3-nitrophenyl)- (9CI) (CA INDEX NAME)



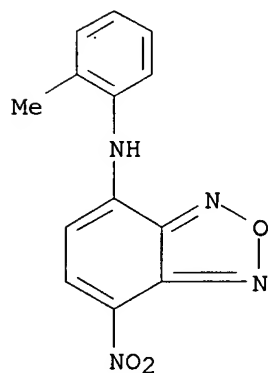
RN 97346-17-3 HCAPLUS

CN 2,1,3-Benzoxadiazol-4-amine, 5,7-dinitro-N-phenyl- (9CI) (CA INDEX NAME)



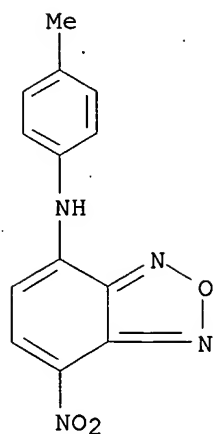
RN 101237-21-2 HCAPLUS

CN 2,1,3-Benzoxadiazol-4-amine, N-(2-methylphenyl)-7-nitro- (9CI) (CA INDEX NAME)



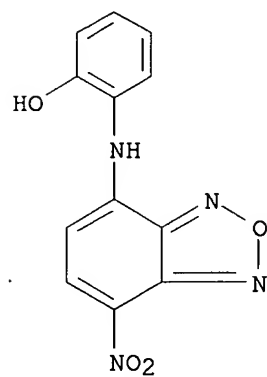
RN 101237-22-3 HCAPLUS

CN 2,1,3-Benzoxadiazol-4-amine, N-(4-methylphenyl)-7-nitro- (9CI) (CA INDEX NAME)



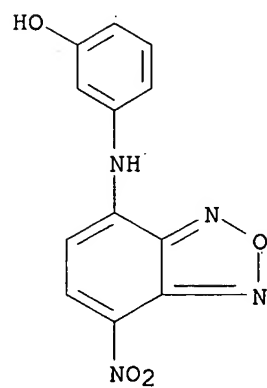
RN 101237-23-4 HCAPLUS

CN Phenol, 2-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]- (9CI) (CA INDEX NAME)

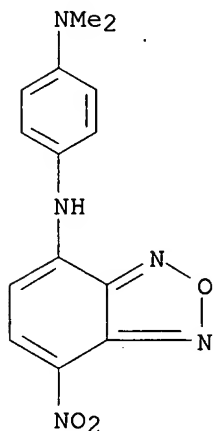


RN 101237-24-5 HCAPLUS

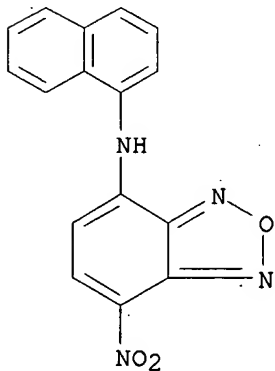
CN Phenol, 3-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]- (9CI) (CA INDEX NAME)



RN 101237-27-8 HCAPLUS

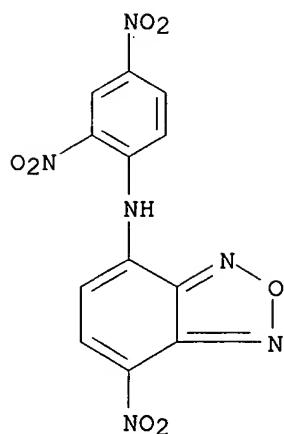
CN 1,4-Benzenediamine, N,N-dimethyl-N'-(7-nitro-2,1,3-benzoxadiazol-4-yl)-  
(9CI) (CA INDEX NAME)

RN 102565-92-4 HCAPLUS

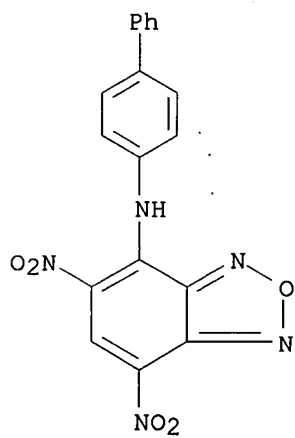
CN 2,1,3-Benzoxadiazol-4-amine, N-1-naphthalenyl-7-nitro- (9CI) (CA INDEX  
NAME)

RN 118025-13-1 HCAPLUS

CN 2,1,3-Benzoxadiazol-4-amine, N-(2,4-dinitrophenyl)-7-nitro- (9CI) (CA  
INDEX NAME)

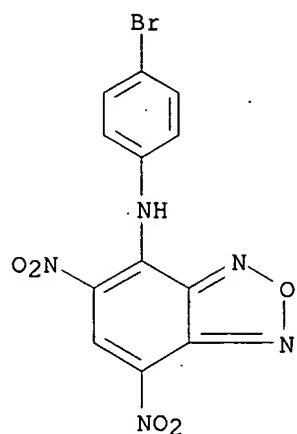


RN 121782-85-2 HCAPLUS

CN 2,1,3-Benzoxadiazol-4-amine, N-[1,1'-biphenyl]-4-yl-5,7-dinitro- (9CI)  
(CA INDEX NAME)

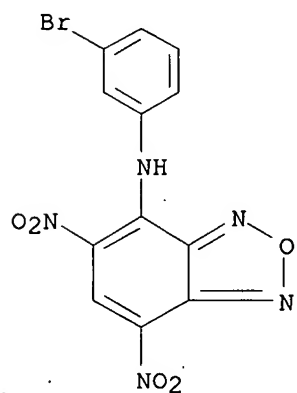
RN 121782-87-4 HCAPLUS

CN 2,1,3-Benzoxadiazol-4-amine, N-(4-bromophenyl)-5,7-dinitro- (9CI) (CA  
INDEX NAME)



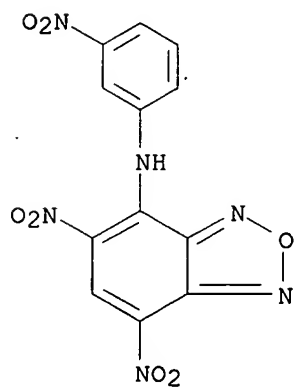
RN 121782-88-5 HCAPLUS

CN 2,1,3-Benzoxadiazol-4-amine, N-(3-bromophenyl)-5,7-dinitro- (9CI) (CA INDEX NAME)



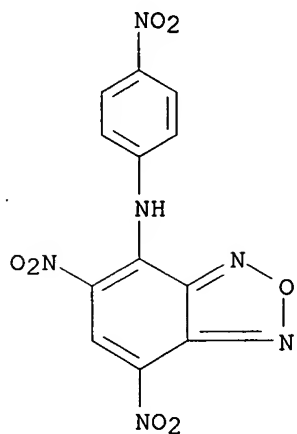
RN 121782-92-1 HCAPLUS

CN 2,1,3-Benzoxadiazol-4-amine, 5,7-dinitro-N-(3-nitrophenyl)- (9CI) (CA INDEX NAME)



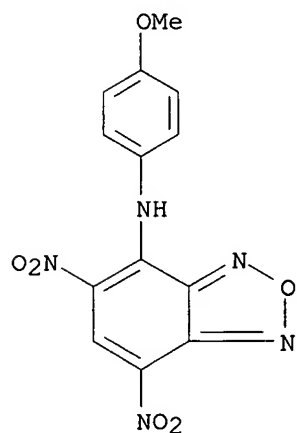
RN 121782-93-2 HCAPLUS

CN 2,1,3-Benzoxadiazol-4-amine, 5,7-dinitro-N-(4-nitrophenyl)- (9CI) (CA INDEX NAME)



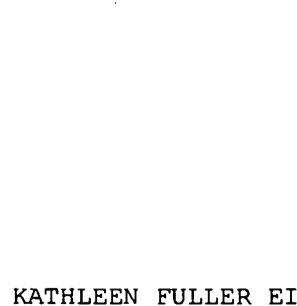
RN 126865-59-6 HCAPLUS

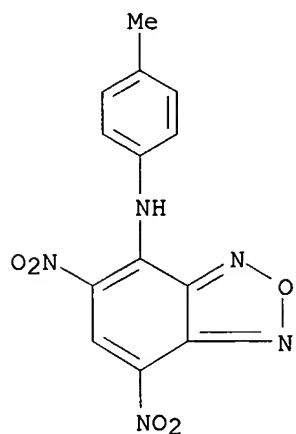
CN 2,1,3-Benzoxadiazol-4-amine, N-(4-methoxyphenyl)-5,7-dinitro- (9CI) (CA INDEX NAME)



RN 126865-60-9 HCAPLUS

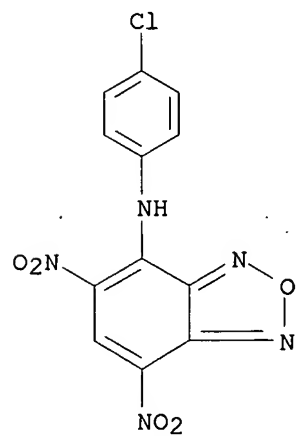
CN 2,1,3-Benzoxadiazol-4-amine, N-(4-methylphenyl)-5,7-dinitro- (9CI) (CA INDEX NAME)





RN 126865-61-0 HCAPLUS

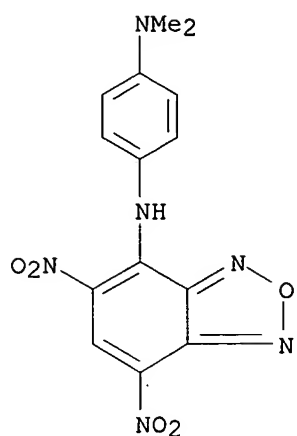
CN 2,1,3-Benzoxadiazol-4-amine, N-(4-chlorophenyl)-5,7-dinitro- (9CI) (CA INDEX NAME)



RN 126865-63-2 HCAPLUS

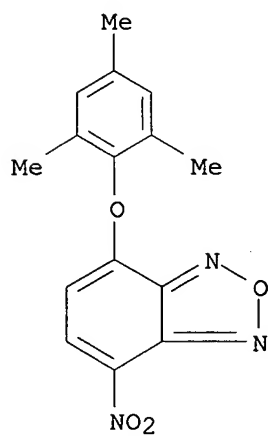
CN 1,4-Benzenediamine, N'-(5,7-dinitro-2,1,3-benzoxadiazol-4-yl)-N,N-dimethyl- (9CI) (CA INDEX NAME)





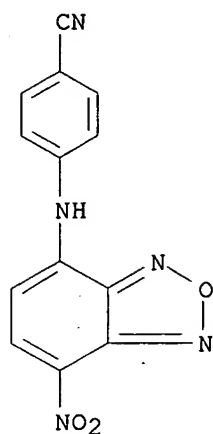
RN 155866-58-3 HCAPLUS

CN 2,1,3-Benzoxadiazole, 4-nitro-7-(2,4,6-trimethylphenoxy)- (9CI) (CA INDEX NAME)



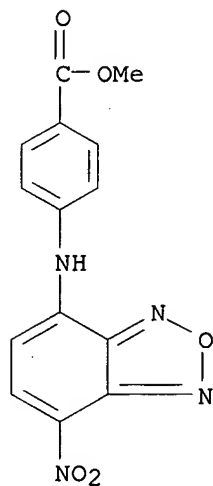
RN 199727-69-0 HCAPLUS

CN Benzonitrile, 4-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]- (9CI) (CA INDEX NAME)



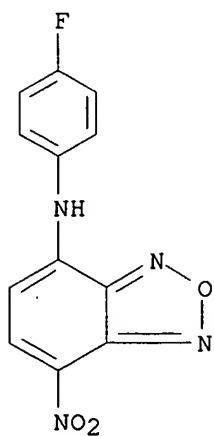
RN 199727-70-3 HCAPLUS

CN Benzoic acid, 4-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]-, methyl ester  
(9CI) (CA INDEX NAME)

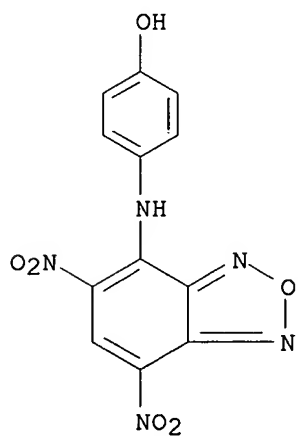


RN 199727-71-4 HCAPLUS

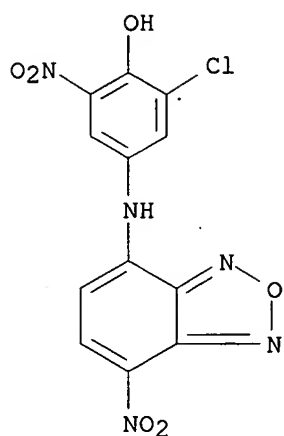
CN 2,1,3-Benzoxadiazol-4-amine, N-(4-fluorophenyl)-7-nitro- (9CI) (CA INDEX NAME)



RN 324525-87-3 HCAPLUS  
CN Phenol, 4-[(5,7-dinitro-2,1,3-benzoxadiazol-4-yl)amino]- (9CI) (CA INDEX NAME)

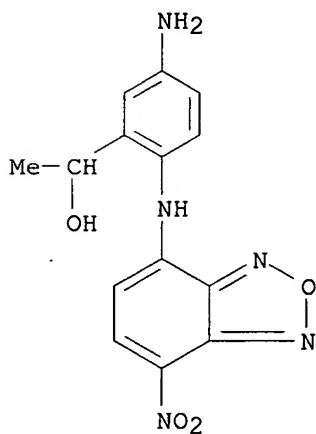


RN 404823-74-1 HCAPLUS  
CN Phenol, 2-chloro-6-nitro-4-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]- (9CI) (CA INDEX NAME)



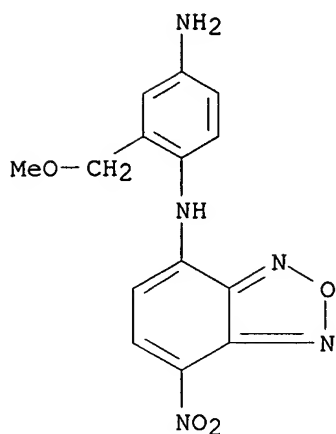
RN 404823-79-6 HCAPLUS

CN Benzenemethanol, 5-amino-.alpha.-methyl-2-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]- (9CI) (CA INDEX NAME)



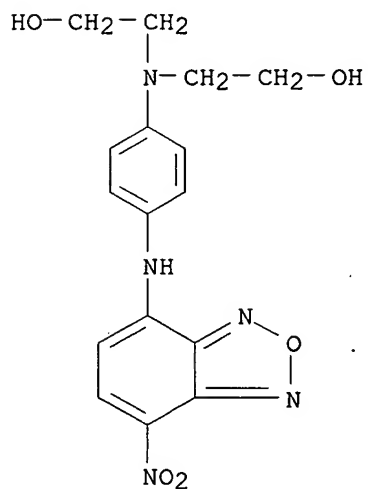
RN 404823-80-9 HCAPLUS

CN 1,4-Benzenediamine, 2-(methoxymethyl)-N1-(7-nitro-2,1,3-benzoxadiazol-4-yl)- (9CI) (CA INDEX NAME)



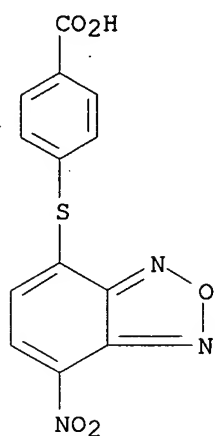
RN 404823-81-0 HCAPLUS

CN Ethanol, 2,2'-[[4-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]phenyl]imino]bis- (9CI) (CA INDEX NAME)



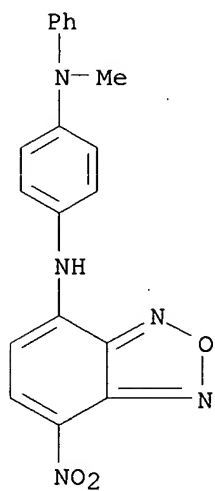
RN 404823-86-5 HCAPLUS

CN Benzoic acid, 4-[(7-nitro-2,1,3-benzoxadiazol-4-yl)thio]- (9CI) (CA INDEX NAME)



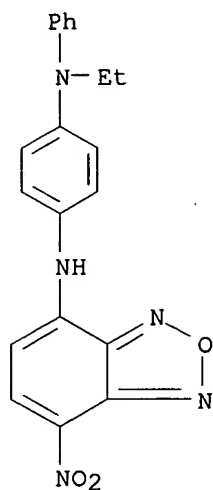
RN 404823-87-6 HCAPLUS

CN 1,4-Benzenediamine, N-methyl-N'-(7-nitro-2,1,3-benzoxadiazol-4-yl)-N-phenyl- (9CI) (CA INDEX NAME)



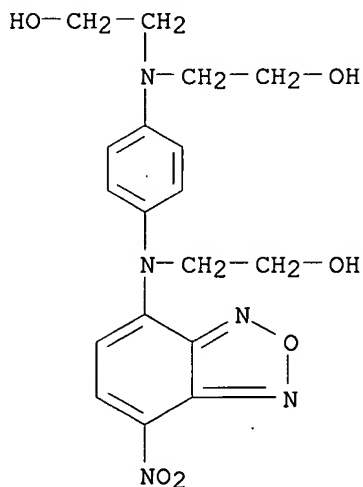
RN 404823-88-7 HCAPLUS

CN 1,4-Benzenediamine, N-ethyl-N'-(7-nitro-2,1,3-benzoxadiazol-4-yl)-N-phenyl- (9CI) (CA INDEX NAME)



RN 404823-89-8 HCAPLUS

CN Ethanol, 2,2'-[[4-[(2-hydroxyethyl)(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]phenyl]imino]bis- (9CI) (CA INDEX NAME)



IT 16597-10-7P 18333-73-8P 18378-15-9P

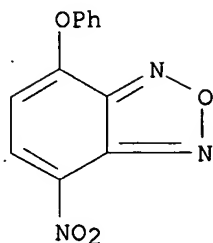
101237-25-6P 101237-26-7P 404823-73-0P

RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(use of 4-nitro-2,1,3-benzoxadiazole derivs. as **hair** dyes)

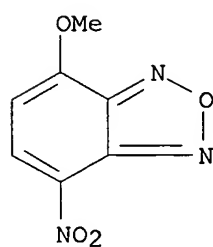
RN 16597-10-7 HCAPLUS

CN 2,1,3-Benzoxadiazole, 4-nitro-7-phenoxy- (9CI) (CA INDEX NAME)



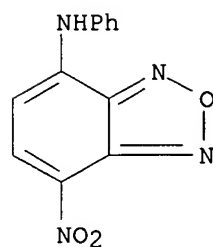
RN 18333-73-8 HCAPLUS

CN 2,1,3-Benzoxadiazole, 4-methoxy-7-nitro- (9CI) (CA INDEX NAME)



RN 18378-15-9 HCAPLUS

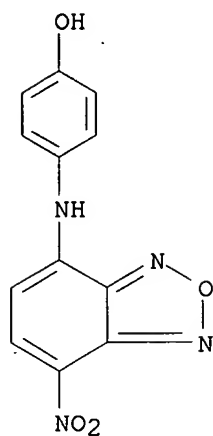
CN 2,1,3-Benzoxadiazol-4-amine, 7-nitro-N-phenyl- (9CI) (CA INDEX NAME)



RN 101237-25-6 HCAPLUS

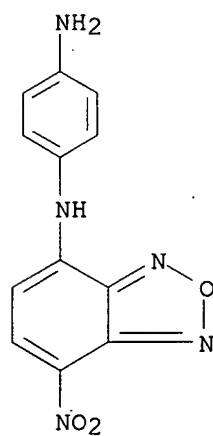
CN Phenol, 4-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]- (9CI) (CA INDEX NAME)





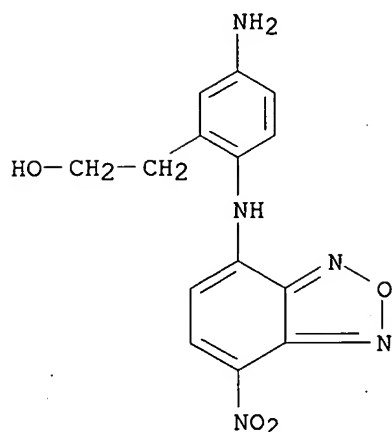
RN 101237-26-7 HCAPLUS

CN 1,4-Benzenediamine, N-(7-nitro-2,1,3-benzoxadiazol-4-yl)- (9CI) (CA INDEX NAME)



RN 404823-73-0 HCAPLUS

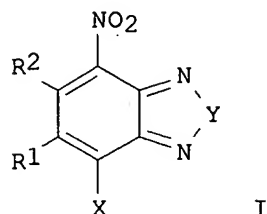
CN Benzeneethanol, 5-amino-2-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]- (9CI) (CA INDEX NAME)



L32 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2003 ACS on STN  
 AN 2002:220343 HCAPLUS  
 DN 136:267891  
 TI **Hair** dyes containing benzoxadiazole, benzothiadiazole and  
 benzo-selenadiazole derivatives  
 IN Pasquier, Cecile; Charriere, Veronique; Braun, Hans-Juergen  
 PA Wella Aktiengesellschaft, Germany  
 SO PCT Int. Appl., 44 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA German  
 IC ICM A61K007-13  
 CC 62-3 (Essential Oils and Cosmetics)  
 Section cross-reference(s): 41

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2002022093	A1	20020321	WO 2001-EP7494	20010629
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG DE 10045600 A1 20020404 DE 2000-10045600 20000915 AU 2001081924 A5 20020326 AU 2001-81924 20010629 BR 2001007215 A 20020709 BR 2001-7215 20010629 EP 1328244 A1 20030723 EP 2001-960429 20010629 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR US 2003070239 A1 20030417 US 2002-110116 20020405 PRAI DE 2000-10045600 A 20000915 WO 2001-EP7494 W 20010629 GI				



AB The invention relates to an agent for coloring fibers (A) which is produced by mixing two components (A1) and (A2) and is characterized in that the component (A1) contains at least one compd. of formula (I), wherein X represents a halogen atom, a methoxy group or an ethoxy group; Y represents an oxygen atom, a sulfuric atom or a selenium atom; and R1 and R2 can be identical or different and represent independently from each other hydrogen, a halogen atom, an (C1-C4) alkyl group, an (C1-C4) alkyl group substituted by a halogen atom, an (C1-C4) alkoxy group, a nitro group, an acetamido group or a NRaRb group, whereby the radicals Ra and Rb can be identical or different and represent independently from each other hydrogen, an (C1-C4) alkyl group, an optionally substituted carbocycle or an (C1-C4) alkane carbonyl group, or Ra and Rb form, together with the nitrogen atom, a heterocyclic (C3-C6) group; and the component (A2) contains at least one compd. from the group comprising amines, aminonitrobenzenes and phenoles. The invention also relates to a method for coloring **hair** by using the agent and a multiple component kit. Thus a **hair** dye was prepd. Component A1 contained (g): 7-chloro-4-nitro-2,1,3-benzoxadiazole 0.5; ethanol 5.0; decylpolyglycoside aq. soln. (Plantaren 2000) 4.0; EDTA sodium salt hydrate 0.2; water to 100. Components A2 was 0.153 g ethanol amine.

ST **hair** dye benzoxadiazole benzothiadiazole benzoselenadiazole deriv amine phenol

IT **Hair** preparations

(dyes; **hair** dyes contg. benzoxadiazole, benzothiadiazole and benzo-selenadiazole derivs.)

IT 95-55-6, 2-Aminophenol 99-98-9, 4-Dimethylaminoaniline 106-44-5, 4-Methylphenol, biological studies 106-50-3, 1,4-Diaminobenzene, biological studies 108-45-2, 1,3-Diaminobenzene, biological studies 108-46-3, 1,3-Dihydroxybenzene, biological studies 108-95-2, Phenol, biological studies 123-30-8, 4-Aminophenol 123-31-9, Hydroquinone, biological studies 141-43-5, Ethanol amine, biological studies 525-64-4, 2,7-Diamino fluorene 591-27-5, 3-Aminophenol 1198-27-2, 2-Naphthalenol, 1-amino-,hydrochloride 1953-54-4, 5-Hydroxyindole 2207-29-6 2274-63-7 2835-95-2, 5-Amino-2-methylphenol 2835-99-6, 4-Amino-3-methylphenol 3240-72-0, 5,6-Diamino-2,4-dihydropyrimidine 3523-28-2 4338-98-1 6358-09-4, 2-Amino-6-chloro-4-nitrophenol 6369-59-1, 1,4-Benzenediamine, 2-methyl-, sulfate 10199-89-0, 7-Chloro-4-nitro-2,1,3-benzoxadiazole 15639-38-0 15639-43-7 15944-78-2 16322-19-3 16461-98-6, 1H-Pyrazole-3,4-diamine 18333-73-8 18392-74-0 18392-77-3 18392-78-4, 4-Bromo-5-methyl-7-nitro-2,1,3-benzothiadiazole 18453-42-4 19951-28-1 19951-33-8 20718-28-9 20718-47-2 20718-48-3 23920-15-2 26455-21-0 26460-78-6 29270-56-2, 4-Fluoro-7-nitro-2,1,3-benzoxadiazole 29705-39-3 32014-70-3 33229-34-4 35128-56-4 45514-38-3, 4,5-Diamino-1-methyl-1H-pyrazole 49647-58-7,

2,4,5,6-Tetraaminopyrimidine sulfate 52120-98-6 56932-44-6  
62625-14-3 65235-31-6, 4-[(2-Hydroxyethyl)amino]-3-nitrophenol  
66170-46-5, 1,4-Benzenediamine, 2-methyl-, hydrochloride 68579-76-0  
69825-83-8 70643-19-5, 2,4-Diamino-1-(2-hydroxyethoxy)benzene  
70733-34-5 71005-35-1 **81432-10-2** 81892-72-0,  
1,3-Di(2,4-diaminophenoxy)propane 83763-47-7, 2-Amino-4-[(2-  
hydroxyethyl)amino]anisole 89365-28-6 89365-31-1 89365-32-2  
89793-88-4 90841-38-6 91267-92-4 93841-24-8, 1,4-Diamino-2-(2-  
hydroxyethyl)benzene 93841-25-9 94158-13-1 95576-89-9 100418-33-5,  
4-[(2-Hydroxyethyl)amino]-3-nitro-1-methylbenzene 104516-93-0  
125292-42-4 131202-67-0 131202-71-6 131311-66-5 131657-78-8,  
2-Chloro-6-ethylamino-4-nitrophenol 132885-85-9 155601-16-4  
155601-17-5, 4,5-Diamino-1-(2-hydroxyethyl)-1H-pyrazole 157469-54-0  
164919-03-3 227199-11-3 257932-06-2 257932-07-3 329320-36-7,  
1,4-Diamino-2-(1-hydroxyethyl)benzene 364343-79-3 404839-62-9  
404839-63-0 404839-64-1

RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)  
(**hair** dyes contg. benzoxadiazole, benzothiadiazole and  
benzo-selenadiazole derivs.)

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD  
RE

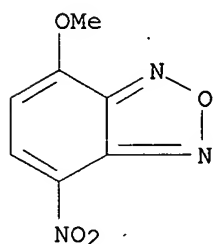
- (1) Bachmann, H; US 4620850 A 1986 HCAPLUS
- (2) Botta, N; US 5055110 A 1991 HCAPLUS
- (3) Oberkobusch, D; WO 0110379 A 2001 HCAPLUS
- (4) Oberkobusch, D; WO 0147485 A 2001
- (5) Pilgram, K; US 3577427 A 1971 HCAPLUS

IT **18333-73-8 81432-10-2**

RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)  
(**hair** dyes contg. benzoxadiazole, benzothiadiazole and  
benzo-selenadiazole derivs.)

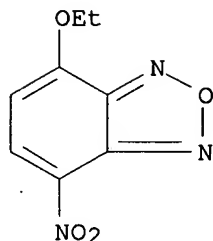
RN 18333-73-8 HCAPLUS

CN 2,1,3-Benzoxadiazole, 4-methoxy-7-nitro- (9CI) (CA INDEX NAME)



RN 81432-10-2 HCAPLUS

CN 2,1,3-Benzoxadiazole, 4-ethoxy-7-nitro- (9CI) (CA INDEX NAME)



L32 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2003 ACS on STN

AN 2000:368704 HCAPLUS

DN 133:14300

TI In situ method of analyzing cells by staining with multiple stains and using a spectral data collection device

IN Garini, Yuval; Mcnamara, George; Soenksen, Dirk G.; Cabib, Dario; Buckwald, Robert A.

PA Applied Spectral Imaging Ltd., Israel

SO PCT Int. Appl., 129 pp.

CODEN: PIXXD2

DT Patent

LA English

IC ICM G01N033-53

ICS C12Q001-54; C12Q001-28; C12Q001-00; C12Q001-42

CC 9-4 (Biochemical Methods)

Section cross-reference(s): 3, 14

FAN.CNT 6

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000031534	A1	20000602	WO 1999-US27000	19991116
	W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	DE 29624210	U1	20010628	DE 1996-29624210	19961210
	US 6165734	A	20001226	US 1998-196690	19981120
	EP 1131631	A1	20010912	EP 1999-963904	19991116
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	JP 2002530676	T2	20020917	JP 2000-584297	19991116
PRAI	US 1998-196690	A	19981120		
	US 1995-571047	A1	19951212		
	EP 1996-944834	A	19961210		
	US 1998-122704	A2	19980727		
	WO 1999-US27000	W	19991116		

AB A method of in situ anal. of a biol. sample comprises the steps of (a) staining the biol. sample with N stains of which a first stain is selected from the group consisting of a first immunohistochem. stain, a first histol. stain and a first DNA ploidy stain, and a second stain is selected from the group consisting of a second immunohistochem. stain, a second

histol. stain and a second DNA ploidy stain, with provisions that N is an integer greater than three and further that (i) if the first stain is the first immunohistochem. stain then the second stain is either the second histol. stain or the second DNA ploidy stain; (ii) if the first stain is the first histol. stain then the second stain is either the second immunohistochem. stain or the second DNA ploidy stain; whereas (iii) if the first stain is the first DNA ploidy stain then the second stain is either the second immunohistochem. stain or the second histol. stain; and (b) using a spectral data collection device for collecting spectral data from the biol. sample, the spectral data collection device and the N stains are selected so that a spectral component assocd. with each of the N stains is collectible. Figure (1) shows a block diagram illustrating the main components of an imaging spectrometer. Breast cancer tissue samples were stained with two histol. stains (hematoxylin and eosin), and four immunohistochem. stains (DAB, AEC, Fast Red, and BCIP/NBT) and measured using the Spectracube system.

ST cell analysis immunohistochem histochem DNA ploidy stain; imaging spectrometer cell analysis staining

IT Dyes

(Alexa; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Antigens

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(CA 15-3, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT CD antigens

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(CD100; antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT CD antigens

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(CD39, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT CD antigens

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(CD9, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT CD antigens

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(CD99, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Proteins, specific or class

RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)

(DNA-binding, fusion protein with green fluorescent protein, as DNA ploidy stain; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Cadherins

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(E-, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Dyes

- (IR, as label; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)
- IT Immunoglobulin receptors  
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
(IgE type II, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)
- IT Blood-group substances  
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
(Lex, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)
- IT Cell adhesion molecules  
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
(PECAM-1, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)
- IT Transcription factors  
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
(Rb, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)
- IT Proteins, specific or class  
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
(S-100, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)
- IT Blood-group substances  
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
(Tn, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)
- IT Cell adhesion molecules  
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
(VCAM-1, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)
- IT Melanosome  
(antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)
- IT CA 125 (carbohydrate antigen)  
CA19-9 antigen  
CD14 (antigen)  
CD19 (antigen)  
CD20 (antigen)  
CD22 (antigen)  
CD3 (antigen)  
CD30 (antigen)  
CD34 (antigen)  
CD38 (antigen)  
CD4 (antigen)  
CD45 (antigen)  
CD45RA (antigen)  
CD45RO (antigen)  
CD5 (antigen)  
CD7 (antigen)  
CD8 (antigen)

Carcinoembryonic antigen  
Epidermal growth factor receptors  
Estrogen receptors  
Fas antigen  
Fibrins

**Keratins**

Ki-67 antigen  
P-glycoproteins  
Progesterone receptors  
Proliferating cell nuclear antigen  
Prostate-specific antigen  
Ras proteins  
Transferrin receptors  
Vimentins

neu (receptor)

p53 (protein)

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Integrins

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(antigens CD11c, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Aequorins

Biliproteins

Enzymes, biological studies

Heavy metals

Phycoerythrins

RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)

(as label; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Fluorescent substances

(as labels; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Proteins, specific or class

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(bcl-2, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Transcription factors

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(c-myc, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Uterus, neoplasm

(cervix, pap smear of; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Avidins

RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)

(conjugates, in signal amplification system; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Staining, biological



## Stains, biological

(fluorescent; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

## IT Proteins, specific or class

RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)

(green fluorescent, fusion protein with DNA-binding protein, as DNA ploidy stain; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

## IT Proteins, specific or class

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(human papillomavirus, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

## IT Chromosome

(human, DNA probes for, labeled with fluorophores; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

## IT Immunoassay

(immunohistochem.; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

## IT Antibodies

RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); PROC (Process); USES (Uses)

(in immunohistochem. staining; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

## IT Avidins

RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)

(in signal amplification system; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

## IT Algorithm

Animal tissue

Biological materials

Cell

Colorimetry

Fluorescent dyes

Histochemistry

Imaging

Interferometry

Luminescence

Optical dispersion

Optical filters

Ploidy

Spectroscopy

Staining, biological

Stains, biological

(in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

## IT Nucleic acid hybridization

(in situ, fluorescence; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

## IT Antibodies

RL: ARG (Analytical reagent use); BPR (Biological process); BSU

- (Biological study, unclassified); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); PROC (Process); USES (Uses) (labeled; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)
- IT Immunoglobulins  
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
(light chains, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)
- IT Mammary gland  
(neoplasm, tissue; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)
- IT Fusion proteins (chimeric proteins)  
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)  
(of DNA binding protein and green fluorescent protein, as DNA ploidy stain; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)
- IT DNA  
RL: BSU (Biological study, unclassified); BIOL (Biological study)  
(ploidy, stain for; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)
- IT Human papillomavirus  
(proteins of, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)
- IT Antigens  
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
(tau, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)
- IT Prostate gland  
Uterus  
(tissue of; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)
- IT Complement receptors  
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
(type 1, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)
- IT Microscopy  
(with Spectracube system; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)
- IT Fluorescent substances  
(with high affinity for DNA, as DNA ploidy stain; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)
- IT Integrins  
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
(.alpha.IIb, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)
- IT 846-70-8, Naphthol yellow S  
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)  
(Feulgen reaction, as histol. stain; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

- device)
- IT 9025-26-7, Cathepsin D 9054-63-1, CD antigens, cd13 60267-61-0, Ubiquitin 71208-06-5, Lewis X 82707-54-8, CD10 (antigen)  
 RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
 (antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)
- IT 65-61-2, Acridine Orange 1239-45-8, Ethidium Bromide 7059-24-7, Chromomycin A 3  
 RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)  
 (as DNA ploidy stain; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)
- IT 83-89-6, Quinacrine 25535-16-4, Propidium Iodide  
 RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)  
 (as histol. stain, as DNA ploidy stain; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)
- IT 61-73-4, Methylene Blue 92-32-0 553-24-2, Neutral Red 633-03-4, Ethyl green 635-78-9, Resorufin 2321-07-5D, Fluorescein, reaction product with phalloidin 5141-20-8, Light Green SF 17372-87-1, Eosin 17466-45-4D, Phalloidin, reaction product with fluorescein 23491-45-4, Hoechst 33258 23491-52-3, Hoechst 33342 27072-45-3, Fluorescein isothiocyanate 47165-04-8, 4',6-Diamidino-2-phenylindole 51811-82-6, Giemsa 54327-10-5, Methyl Green 81604-88-8, Orange G  
 RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)  
 (as histol. stain; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)
- IT 53-57-6, NADPH 58-68-4, NADH 60-18-4, L-Tyrosine, biological studies 73-22-3, L-Tryptophan, biological studies 146-14-5, FAD 1461-15-0, Calcein 2321-07-5, Fluorescein 9001-37-0, Glucose oxidase 9001-78-9 9003-99-0, Peroxidase 9014-00-0, Luciferase 9031-11-2, .beta.-Galactosidase 13558-31-1D, derivs. 41085-99-8 53213-83-5, DiOC7(3) 69432-00-4, Calcofluor White 82354-19-6, Texas Red 88235-25-0 98285-52-0, Spectrum Orange 102185-03-5, Cy2 138026-71-8, BODIPY 146368-14-1, Cy5 146368-16-3, Cy3 148504-34-1, Calcein-AM 159501-37-8, Cyclic GDP-Ribose 167095-09-2, MitoTracker Red 169799-14-8, Cy 7 172971-77-6 172971-78-7 189767-45-1, Cy 3.5 189767-52-0, FluorX 195395-80-3, Spectrum Green 220356-37-6, VECTOR Red 223786-97-8, Spectrum Aqua 272457-05-3, Cy 0 272457-06-4, Cy 0.5 272457-19-9, Cy 1 (dye) 272457-27-9, Cy 1.5 272457-33-7, CryptoFluor S 272457-83-7, Spectrum Blue 272457-89-3, Spectrum Gold 272458-01-2, Spectrum Red  
 RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)  
 (as label; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)
- IT 56-65-5, ATP, biological studies 2591-17-5, Luciferin 7440-70-2, Calcium, biological studies 55779-48-1, Coelenterazine  
 RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)  
 (as substrates; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)
- IT 58-85-5, Biotin  
 RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)

(in signal amplification system; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT 82446-52-4, Lucifer Yellow  
RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); PROC (Process); USES (Uses)  
(in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT 58-85-5D, Biotin, antibody conjugates 298-83-9, NBT 517-28-2, Hematoxylin 1448-16-4, DAB 1672-46-4D, Digoxigenin, conjugates with DNA and rhodamine 6409-77-4, Nuclear Fast Red 7240-90-6, X-Gal 8005-77-4, Bismarck brown Y 9013-20-1D, Streptavidin, antibody conjugates 38404-93-2, BCIP 77045-20-6, Fast Red 272459-19-5, Vecor SG  
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)  
(in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT 2465-27-2, Auramine O 65589-70-0, Acridine  
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)  
(reaction product with Feulgen, as DNA ploidy stain; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT 9013-20-1, Streptavidin  
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)  
(with antibody; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD

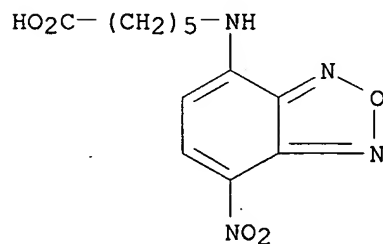
RE

(1) McNamara; US 6007996 A 1999 HCAPLUS

IT 88235-25-0  
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)  
(as label; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

RN 88235-25-0 HCAPLUS

CN Hexanoic acid, 6-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]- (9CI) (CA INDEX NAME)



L32 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2003 ACS on STN

AN 1989:53390 HCAPLUS

DN 110:53390

KATHLEEN FULLER EIC 1700/PARKER LAW 308-4290

- TI Synthesis of pyrenesulfonylamido-sphingomyelin and its use as substrate for determining sphingomyelinase activity and diagnosing Niemann-Pick disease
- AU Klar, Rachel; Levade, Thierry; Gatt, Shimon
- CS Hadassah Sch. Med., Hebrew Univ., Jerusalem, 91010, Israel
- SO Clinica Chimica Acta (1988), 176(3), 259-67  
CODEN: CCATAR; ISSN: 0009-8981
- DT Journal
- LA English
- CC 7-1 (Enzymes)  
Section cross-reference(s): 14
- AB A new fluorescent deriv. of sphingomyelin (PSA 12-sphingomyelin) contg. a pyrene-sulfonylamide residue was synthesized by covalently linking 12-((1-pyrenesulfonyl)amido)-dodecanoic acid (PSA12) to sphingosylphosphorylcholine. It was used as substrate for acidic and neutral human and murine sphingomyelinases, permitting development of sensitive assays for these enzymic activities. The product of the sphingomyelinase assay, PSA12-ceramide, could be detected in picomole quantities due to a fluorescence intensity which was 10-35-fold greater than that of other fluorescent ceramides (such as pyrene or nitrobenzoxadiazole derivs.). PSA 12-sphingomyelin could be used in pure form or admixed with natural sphingomyelin; in the latter case, the enzyme hydrolyzed the fluorescent and non-fluorescent species at equal rates. Use of PSA12-sphingomyelin permitted detn. of sphingomyelinase activity in cell exts. (e.g. human blood lymphocytes, lymphoid cell lines or cultured skin fibroblasts) as well as in **hair** follicles and urine. This new fluorescent deriv. of sphingomyelin also permitted the detection of acid sphingomyelinase deficiency in cells derived from patients with Niemann-Pick disease.
- ST sphingomyelinase detn sphingomyelin fluorescent deriv; Neiman Pick disease sphingomyelinase detn; pyrenesulfonylamidosphingomyelin prepn sphingomyelinase detn
- IT Niemann-Pick disease  
(diagnosis of, in human, detection of acid sphingomyelinase deficiency in)
- IT Michaelis constant  
(of sphingomyelinase, of human skin fibroblasts, with pyrenesulfonylamidododecanoyl sphingosylphosphorylcholine)
- IT Fibroblast  
(sphingomyelinase detn. in human, fluorescent substrate for, in Niemann-Pick disease diagnosis)
- IT Lymphocyte  
(sphingomyelinase detn. in, of human blood, fluorescent substrate for, in Niemann-Pick disease diagnosis)
- IT Lymphoblast  
(sphingomyelinase detn. in, of human skin, fluorescent substrate for, in Niemann-Pick disease diagnosis)
- IT Urine analysis  
(sphingomyelinase detn. in, of human, fluorescent substrate for)
- IT **Hair**  
(follicle, sphingomyelinase detn. in human, fluorescent substrate for)
- IT Sphingomyelins  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(N-[(pyrenylsulfonyl)amino]lauroyl], prepn. and use in sphingomyelinase detn. and Niemann-Pick disease diagnosis)
- IT 9031-54-3, Sphingomyelinase  
RL: BIOL (Biological study)  
(acidic and neutral, detn. of, in human and lab. animal in health and

Niemann-Pick disease, fluorescent substrate for)

IT 118540-32-2  
RL: BIOL (Biological study)  
(condensation of, with pyrenesulfonylamidododecanoic acid)

IT 73025-01-1 111864-04-1  
RL: BIOL (Biological study)  
(condensation of, with sphingosylphosphorylcholine)

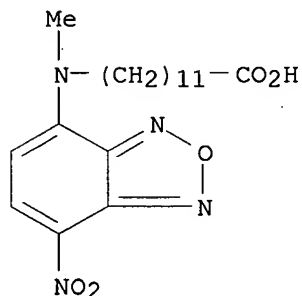
IT 118578-43-1P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and use in human and lab. animal sphingomyelinase detn. in health and Niemann-Pick disease)

IT 118540-33-3P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and use in sphingomyelinase detn. and Niemann-Pick disease diagnosis)

IT 73025-01-1  
RL: BIOL (Biological study)  
(condensation of, with sphingosylphosphorylcholine)

RN 73025-01-1 HCAPLUS

CN Dodecanoic acid, 12-[methyl(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]- (9CI)  
(CA INDEX NAME)

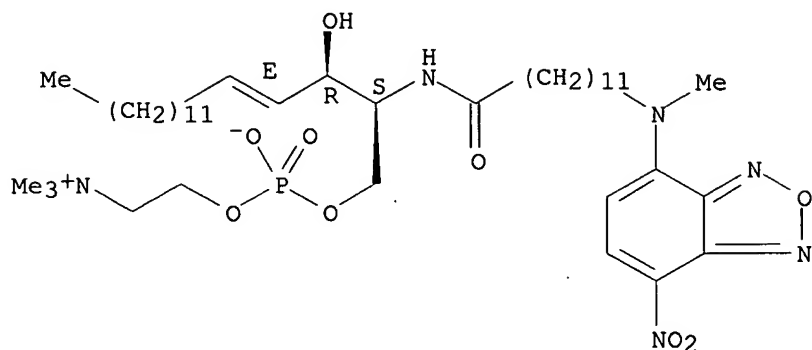


IT 118540-33-3P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and use in sphingomyelinase detn. and Niemann-Pick disease diagnosis)

RN 118540-33-3 HCAPLUS

CN 18,20-Dioxa-2,15-diaza-19-phosphadocosan-22-aminium, 19-hydroxy-16-(1-hydroxy-2-pentadecenyl)-N,N,N-trimethyl-2-(7-nitro-2,1,3-benzoxadiazol-4-yl)-14-oxo-, inner salt, 19-oxide, [R-[R\*,S\*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.



L32 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2003 ACS on STN

AN 1988:607706 HCAPLUS

DN 109:207706

TI In situ localization of actin filaments in higher plant cells using fluorescent probes

AU Parthasarathy, M. V.

CS Div. Biol. Sci., Cornell Univ., Ithaca, NY, 14853, USA

SO Plant Molecular Biology Reporter (1987), 5(1), 251-9

CODEN: PMBRD4; ISSN: 0735-9640

DT Journal

LA English

CC 9-4 (Biochemical Methods)

Section cross-reference(s): 11

AB Procedures for the in situ localization of F-actin in various plant tissues, pollen, and tissue cultured cells are described, using rhodamine-phalloidin (Rh-Ph) as the fluorescent probe. 7-Nitroben-2-oxa-1,3-diazole-phalloidin can also be used as a probe, but it tends to fade faster than Rh-Ph during observation and photog. Photomicrographs indicate that actin filaments form a three-dimensional network with fine branches extending into the crit. region of the cell. F-actin is often assocd. with the nucleus and frequently appears to terminate at or near the plasma membrane. The architecture of F-actin varies, depending on the cell shape.

ST actin filament plant cell; fluorescence microscopy actin filament plant cell

IT Tobacco

(actin filament localization in cells of, fluorescent probes in evaluation of)

IT Barley

Oat

(actin filament localization in coleoptile cells of, fluorescent probes in evaluation of)

IT Cytoskeleton

Pollen

(actin localization in, fluorescent probes in evaluation of)

IT Tomato

(actin-filament localization in stem hair cells of, fluorescent probes in evaluation of)

IT Actins

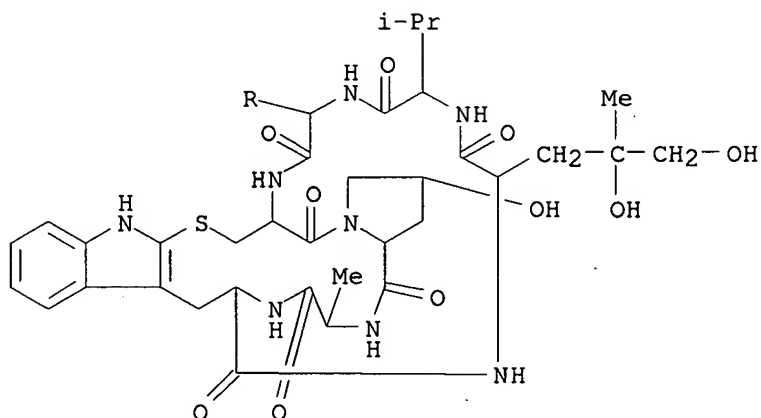
RL: PROC (Process)

(F-, localization of, in plant cells with fluorescent probes)

IT Microscopy

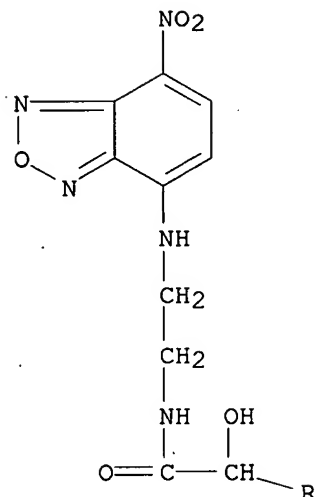
(fluorescence, in actin filament localization in plant cells)  
IT Fluorescent substances  
(probes, actin filament localization in plant cells evaluation by)  
IT Plant tissue culture  
(suspension, of carrot and tobacco, actin filament localization in  
cells of, fluorescent probes in evaluation of)  
IT 509-72-8D, reaction products with phalloidin 17466-45-4D, reaction  
products with rhodamine **73413-78-2**  
RL: ANST (Analytical study)  
(actin filament localization in plant cells evaluation by)  
IT **73413-78-2**  
RL: ANST (Analytical study)  
(actin filament localization in plant cells evaluation by)  
RN 73413-78-2 HCAPLUS  
CN Phalloidin, 5-[erythro-3-hydroxy-N-[2-[(7-nitro-2,1,3-benzoxadiazol-4-  
yl)amino]ethyl]-D-asparagine]- (9CI) (CA INDEX NAME)

PAGE 1-A





PAGE 2-A



L32 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2003 ACS on STN  
AN 1981:180484 HCAPLUS  
DN 94:180484  
TI High pressure liquid chromatography determination of thioglycolic acid in cold wave fluids and depilating creams  
AU Rooselaar, J.; Liem, D. H.  
CS Food Inspection Serv. Enschede, Enschede, 7500 AT, Neth.  
SO International Journal of Cosmetic Science (1981), 3(1), 37-47  
CODEN: IJCMDW; ISSN: 0142-5463  
DT Journal  
LA English  
CC 62-1 (Essential Oils and Cosmetics)  
AB In a high-pressure liq. chromatog. method for the detn. of thioglycolic acid [68-11-1] in **hair** waving fluids and depilatories, the acid is converted to a yellow nitrobenzoxadiazole (NBD) deriv. before chromatog. to permit detection at 464 nm. Optimum derivatization conditions could be obtained when 0.01% aq. solns. of thioglycolic acid were heated with 7-chloro-4-nitrobenz-2-oxa-1,3-diazole [10199-89-0] at pH 7. **Hair** waving fluids and depilatories are simply dild. with an aq. pH 7 buffer and, if necessary, clarified and filtered, before the derivatization procedure. An internal std., Sunset Yellow FCF, is added to the mixt. before performing ion-pair reverse-phase HPLC. A reverse phase C18 column is used. The mobile phase is aq. MeOH, to which the counter ion, tetrabutylammonium phosphate, is added. Recoveries were 97.8-100.7%. The proposed method permits a resolu. of other mercapto compds., such as thiolactic acid [79-42-5] and thioglycerol [96-27-5]. Sixty market samples of cold wave fluids and depilatories were analyzed by the proposed method, and the results were generally lower than those obtained by iodometric titrn.  
ST thioglycolate detn depilatory **hair** waving; high pressure liq chromatog thioglycolate; nitrobenzoxadiazolethioglycolate chromatog  
IT Depilatories  
(thioglycolic acid detn. in, by high-pressure liq. chromatog.)  
IT Chromatography, column and liquid  
(high-pressure, of nitrobenzoxadiazole mercapto derivs.)

IT **Hair preparations**  
(wave-setting, thioglycolic acid detn. in, by high-pressure liq. chromatog.)

IT 79-42-5 96-27-5 107-96-0  
RL: ANT (Analyte); ANST (Analytical study)  
(detn. of, by high-pressure liq. chromatog.)

IT 68-11-1, analysis  
RL: ANT (Analyte); ANST (Analytical study)  
(detn. of, in depilatories and **hair**-waving solns. by high-pressure liq. chromatog.)

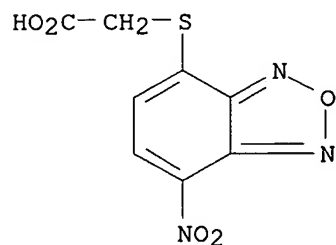
IT **18333-81-8P 77460-15-2P 77460-16-3P 77460-17-4P**  
RL: PREP (Preparation)  
(prepn. of, for high-pressure liq. chromatog.)

IT 10199-89-0  
RL: BIOL (Biological study)  
(reaction with mercapto compds., for high-pressure liq. chromatog. anal.)

IT **18333-81-8P 77460-15-2P 77460-16-3P 77460-17-4P**  
RL: PREP (Preparation)  
(prepn. of, for high-pressure liq. chromatog.)

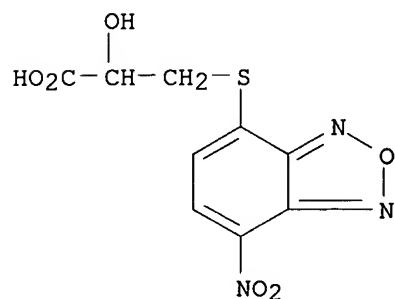
RN 18333-81-8 HCAPLUS

CN Acetic acid, [(7-nitro-2,1,3-benzoxadiazol-4-yl)thio]- (9CI) (CA INDEX NAME)



RN 77460-15-2 HCAPLUS

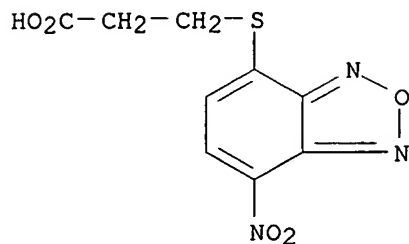
CN Propanoic acid, 2-hydroxy-3-[(7-nitro-2,1,3-benzoxadiazol-4-yl)thio]- (9CI) (CA INDEX NAME)



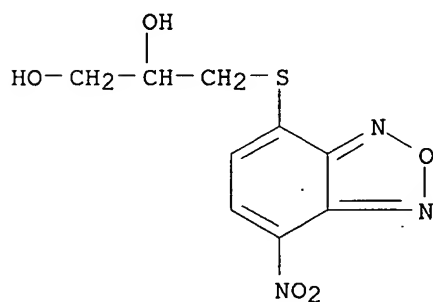
RN 77460-16-3 HCAPLUS

CN Propanoic acid, 3-[(7-nitro-2,1,3-benzoxadiazol-4-yl)thio]- (9CI) (CA

INDEX NAME)



RN 77460-17-4 HCAPLUS

CN 1,2-Propanediol, 3-[(7-nitro-2,1,3-benzoxadiazol-4-yl)thio]- (9CI) (CA  
INDEX NAME)

L32 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2003 ACS on STN

AN 1980:123835 HCAPLUS

DN 92:123835

TI A fluorometric determination of sphingomyelinase by use of fluorescent derivatives of sphingomyelin, and its application to diagnosis of Niemann-Pick disease

AU Gatt, S.; Dinur, T.; Barenholz, Y.

CS Hadassah Med. Sch., Hebrew Univ., Jerusalem, Israel

SO Clinical Chemistry (Washington, DC, United States) (1980), 26(1), 93-6  
CODEN: CLCHAU; ISSN: 0009-9147

DT Journal

LA English

CC 7-1 (Enzymes)

Section cross-reference(s): 14

AB Fluorescent derivs. of sphingomyelin (N-acylsphingosylphosphocholine) were synthesized and used as substrates for several sphingomyelinase (I) preps. The following 5 fluorescent probes, each attached to the terminal C atom of the fatty acyl residue, were introduced into sphingomyelin: dansyl, pyrene, carbazole, 4-chloro-7-nitrobenz-2-oxa-1,3-diazole, and anthroic acid. The rates at which the fluoro- and radiolabeled sphingomyelins were hydrolyzed were detd. The rates were the same with these 3 I preps.: (a) a purified I from *Staphylococcus aureus*; (b) a Triton X-100-treated ext. of human brain (assayed at pH 7.4 in the presence of Mg<sup>2+</sup>); and (c) aq. exts. of brain lysosomes, skin fibroblasts, and amniotic cells, assayed at pH 5.0. Homogenates of skin fibroblasts of

a patient with Niemann-Pick disease had practically no activity when assayed at pH 5 with fluorosphingomyelin as substrate. When fluorosphingomyelin was mixed in various proportions with natural sphingomyelin, I from each of the 3 sources hydrolyzed the 2 substrates at equal rates. The fluorosphingomyelins can be used to est. I activity with great sensitivity in exts. of tissues or cells, in tears, and probably in hair follicles, as well as diagnose Niemann-Pick disease, either pre- or postnatally.

- ST sphingomyelinase detn fluorometry; Niemann Pick disease diagnosis  
sphingomyelinase; sphingomyelin fluorescent deriv prepn
- IT Niemann-Pick disease  
(diagnosis of, sphingomyelinase detn. in)
- IT Amniotic fluid  
(sphingomyelinase detn. in cells of, prenatal Nieman-Pick Disease  
diagnosis in relation to)
- IT Fibroblast  
(sphingomyelinase detn. in, Niemann-Pick Disease diagnosis in relation  
to)
- IT Sphingomyelins  
(fluorescent fatty acid-contg., prepn. and use in sphingomyelinase  
detn.)
- IT 60177-21-1 64821-29-0 69168-45-2 73024-99-4 73025-00-0  
73025-01-1 73025-02-2 73038-57-0  
RL: BIOL (Biological study)  
(condensation of, with sphingosylphosphocholine)
- IT 9031-54-3  
RL: ANT (Analyte); ANST (Analytical study)  
(detn. of, fluorometric, in Niemann-Pick Disease diagnosis)
- IT 73025-01-1  
RL: BIOL (Biological study)  
(condensation of, with sphingosylphosphocholine)
- RN 73025-01-1 HCAPLUS
- CN Dodecanoic acid, 12-[methyl(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]- (9CI)  
(CA INDEX NAME)

